STN Structure Search

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:29:51 ON 19 FEB 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:29:58 ON 19 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 FEB 2007 HIGHEST RN 921759-52-6
DICTIONARY FILE UPDATES: 18 FEB 2007 HIGHEST RN 921759-52-6

III → II

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

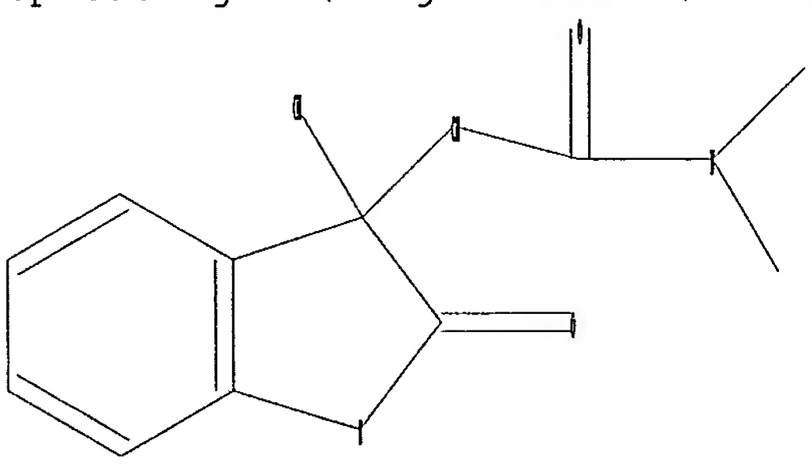
Claim 6

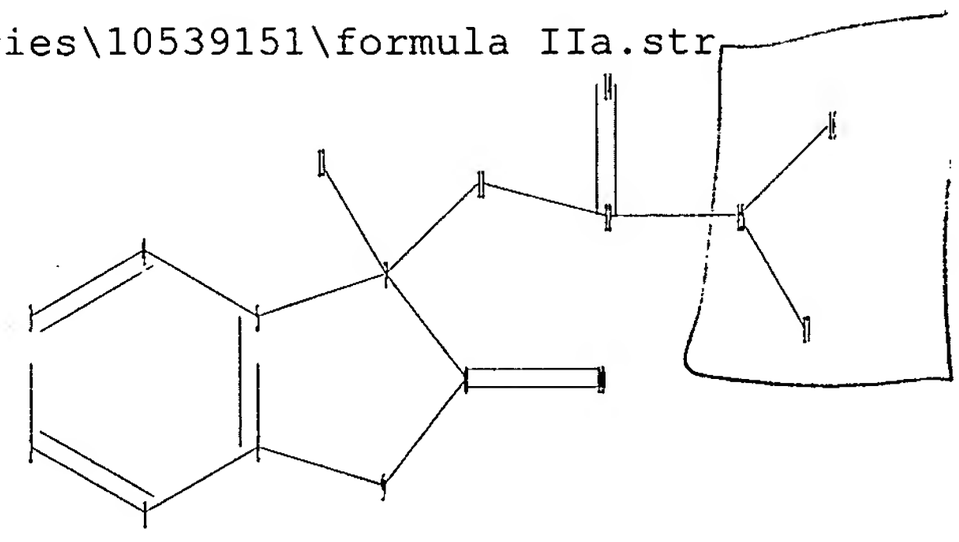
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

Formula II — free of prior art

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\formula IIa.str





ring / chain

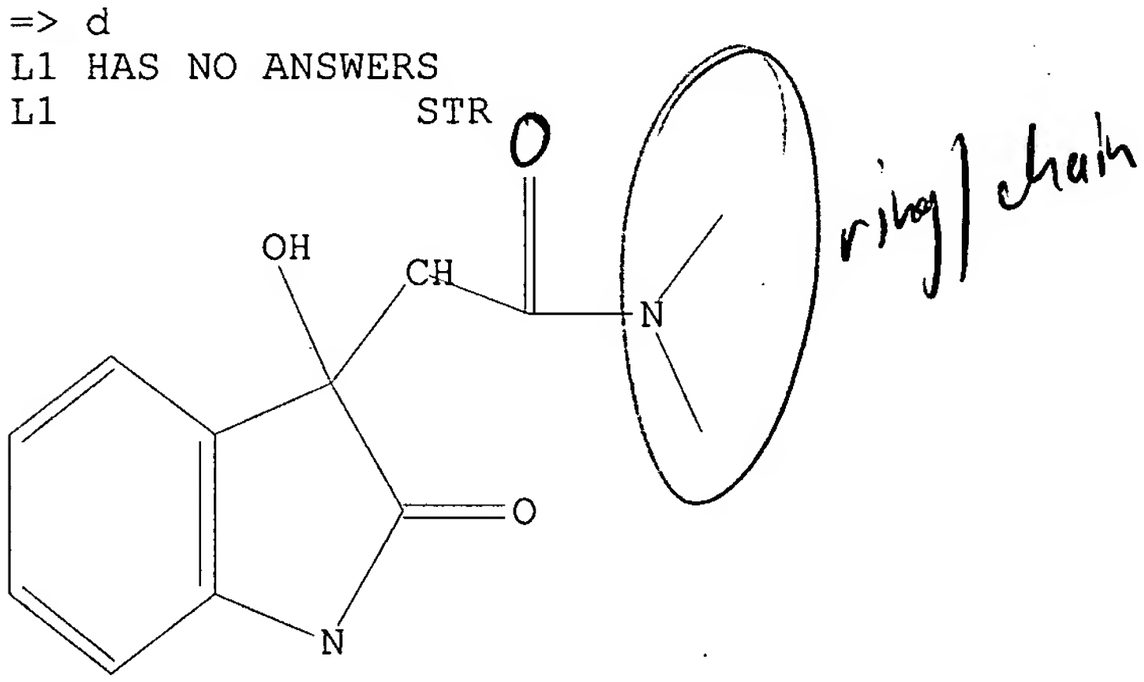
chain nodes :
10 11 12 13 14

ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
15 16 17
chain bonds :
7-11 7-13 8-10 11-12 12-14 12-15
ring/chain bonds :
15-16 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-13 8-9 8-10 12-14 12-15 15-16 15-17
exact bonds :
7-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 10:30:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 782 TO ITERATE

100.0% PROCESSED 782 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

L2 11 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 10:30:34 ON 19 FEB 2007

FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

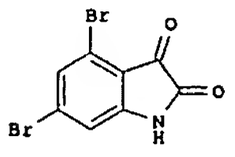
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

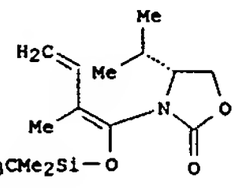
=> s l2
L3 3 L2

=> d ibib abs hitstr 1-3

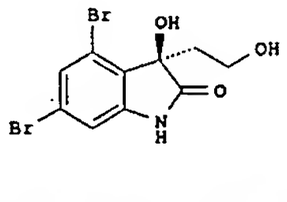
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:49644 CAPLUS
DOCUMENT NUMBER: 144:292911
TITLE: Enantioselective Total Synthesis of Convolutamydines B and E
AUTHOR(S): Nakamura, Tomoaki; Shirokawa, Shinichi; Hosokawa, Seijiro; Nakazaki, Atsuo; Kobayashi, Susumu
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Tokyo University of Science (RIKADAI), Chiba, 278-8510, Japan
SOURCE: Organic Letters (2006), 8(4), 677-679
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:292911
GI



I



II



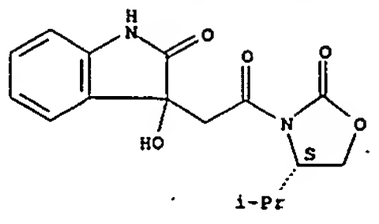
III

AB The first enantioselective total synthesis of convolutamydines B and E has been achieved using our vinylogous Mukaiyama aldol reaction. The synthesis features highly diastereoselective vinylogous Mukaiyama aldol reaction with isatin instead of aldehydes to construct a chiral center of convolutamydines. Thus, isatin I was reacted with N,O-acetal II to give the aldol adduct which was transformed in several steps to (R)-convolutamydine E III. Addnl., the absolute configuration of natural convolutamydine B has been determined as R by its CD spectrum.

IT 879123-17-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. total synthesis of convolutamydines B and E via diastereoselective vinylogous Mukaiyama aldol of isatin derivative)
RN 879123-17-8 CAPLUS
CN 2-Oxazolidinone, 3-[(2,3-dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)acetyl]-4-(1-methylethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

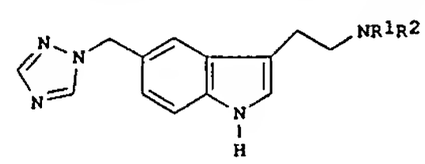
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:811739 CAPLUS
DOCUMENT NUMBER: 143:229863
TITLE: A manufacturing of (triazolylmethyl)indole derivatives and their intermediates
INVENTOR(S): Martin, Pierre; Berens, Ulrich; Boudier, Andreas; Dosenbach, Oliver
PATENT ASSIGNEE(S): Ratiopharm G.m.b.H., Germany
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075422	A1	20050818	WO 2005-EP793	20050127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553652	A1	20050818	CA 2005-2553652	20050127
EP 1751104	A1	20070214	EP 2005-707035	20050127
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				

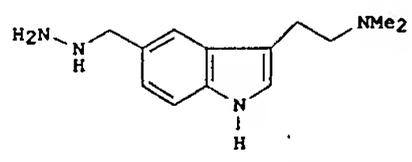
PRIORITY APPLN. INFO.: EP 2004-100303 A 20040128
US 2004-543463P P 20040210
WO 2005-EP793 W 20050127

OTHER SOURCE(S): MARPAT 143:229863
GI

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



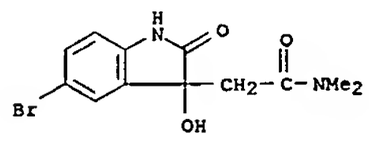
I



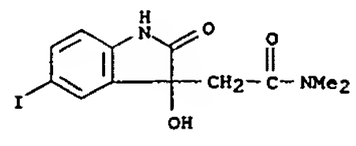
II

AB The invention relates to a preparation of (triazolylmethyl)indole derivs. of formula I [wherein: R1 and R2 are independently H or alkyl] and their intermediates. For instance, anti-migraine agent rizatriptan I [R1 = R2 = Me; no biol. data] was prepared from [(hydrazinomethylindolyl)ethyl]-dimethyl-amine II with a yield of 55%.

IT 717139-78-1P 717139-81-6P 717139-87-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(manufacturing of (triazolylmethyl)indole derivs. and their intermediates)
RN 717139-78-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo- (9CI) (CA INDEX NAME)

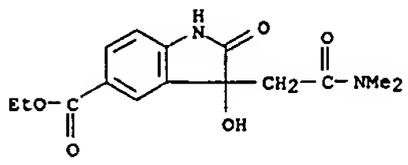


RN 717139-81-6 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-iodo-N,N-dimethyl-2-oxo- (9CI) (CA INDEX NAME)



RN 717139-87-2 CAPLUS
CN 1H-Indole-5-carboxylic acid, yl]-2,3-dihydro-

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
3-hydroxy-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

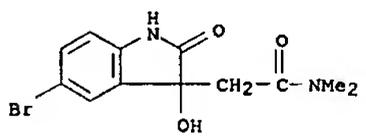
FORMAT

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

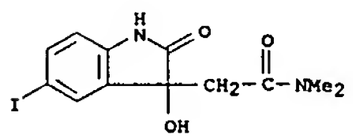
AB Indoleacetates I [R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclyl, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2, CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHNH2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, arylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4] were prepared and converted to I
[R = CONR4R5; R4, R5 = (un)substituted alkyl; R4R5 = (un)substituted alkylene] which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoisatin was treated with CH2(CO2H)2 and ClCONMe2 to give I [R = CONMe2, R1 = 5-Br, R2 = H] which was treated with BF3.Et2O and BH3.Me2SO to give 2-(5-bromo-1H-indol-3-yl)-N,N-dimethylacetamide or with BF3.Et2O and NaBH4 to give [2-(5-bromo-1H-indol-3-yl)ethyl]-N,N-dimethylacetamide.

IT 717139-78-1P 717139-81-6P 717139-88-3P
717139-92-9P 717139-93-0P 717139-95-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tryptamine derivs. and intermediates thereof)

RN 717139-78-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo- (9CI) (CA INDEX NAME)



RN 717139-81-6 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-iodo-N,N-dimethyl-2-oxo- (9CI) (CA INDEX NAME)



RN 717139-88-3 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

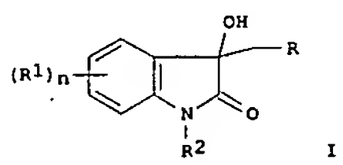
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546477 CAPLUS
DOCUMENT NUMBER: 141:89009
TITLE: Synthesis of tryptamine derivatives and intermediates thereof
INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Instant app

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
WO 2004056769	B1	20041104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2508290	A1	20040708	CA 2003-2508290	20031212
AU 2003299227	A1	20040714	AU 2003-299227	20031212
EP 1572647	A2	20050914	EP 2003-799560	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1729174	A	20060201	CN 2003-80107086	20031212
JP 2006516128	T	20060622	JP 2004-561492	20031212
US 2006058367	A1	20060316	US 2005-539151	20050616

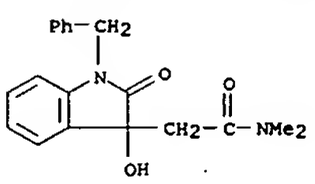
PRIORITY APPLN. INFO.: EP 2002-406128 A 20021220
WO 2003-EP50992 W 20031212

OTHER SOURCE(S): MARPAT 141:89009
GI

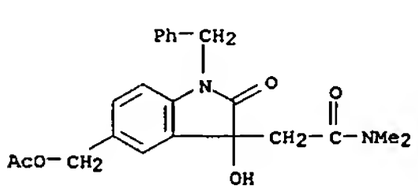


I

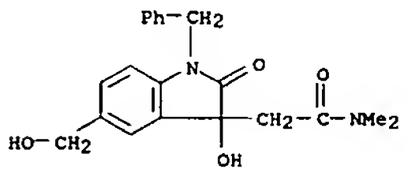
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



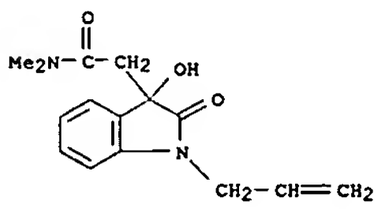
RN 717139-92-9 CAPLUS
CN 1H-Indole-3-acetamide, 5-[(acetyloxy)methyl]-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-93-0 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-(hydroxymethyl)-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



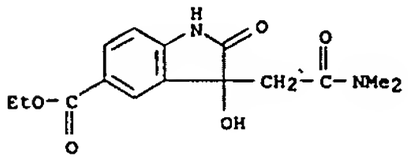
RN 717139-95-2 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(2-propenyl)- (9CI) (CA INDEX NAME)



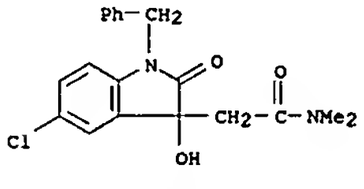
IT 717139-87-2P 717139-91-8P 717139-94-1P
717139-96-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tryptamine derivs. and intermediates thereof)

RN 717139-87-2 CAPLUS

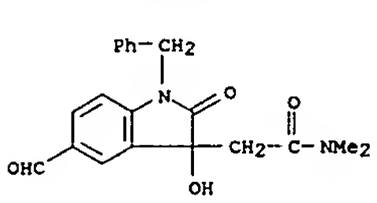
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Indole-5-carboxylic acid,
3-[2-(dimethylamino)-2-oxoethyl]-2,3-dihydro-
3-hydroxy-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 717139-91-8 CAPLUS
CN 1H-Indole-3-acetamide,
5-chloro-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-
(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-94-1 CAPLUS
CN 1H-Indole-3-acetamide,
5-formyl-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-
(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-96-3 CAPLUS
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-(hydroxymethyl)-N,N-
dimethyl-2-oxo-1-(2-propenyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)